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I U C L I D

Data Set

Existing Chemical : ID: 3648-20-2
CAS No. : 3648-20-2
EINECS Name : diundecyl phthalate
EC No. : 222-884-9
TSCA Name : 1,2-Benzenedicarboxylic acid, diundecyl ester
IUPAC Name : diundecyl phthalate
Molecular Formula : C30H50O4

Producer related part

Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Substance related part

Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Status :
Memo : ACC Phthalate Ester Panel HPV Testing Group

Printing date : 07.12.2006
Revision date :
Date of last update : 07.12.2006

Number of pages : 34

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 3648-20-2
Date 07.12.2006

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : ACC Phthalate Esters Panel HPV Testing Group
Contact person : Dr. Marian Stanley
Date :
Street : 1300 Wilson Blvd.
Town : 22209 Arlington, VA
Country : United States
Phone : (703) 741-5623
Telefax : (703) 741-6091
Telex :
Cedex :
Email :
Homepage :

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

01.11.2000

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freetext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and

linear alkyl (B79P)

68515-45-7 1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1. General Information

Id 3648-20-2
Date 07.12.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Polymers industry

Remark : High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 3648-20-2
Date 07.12.2006

2.1 MELTING POINT

Value	:	-9 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Remark	:	<p>Physicochemical data for 18 commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the values for melting point represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate. There were no data on purity. Identified data sources included:</p> <p>Howard P, Banerjee S and Robillard K (1985). Measurement of water solubilities, octanol/water partition coefficients and vapor pressures of commercial phthalate esters. Environ. Tox. Chem 4, 653-661.</p> <p>Howear P (1989). Handbook of Environmental Fate and Exposure Data for Organic Chemicals: Vol I. Large Production and Priority Pollutants. Lewis Publishers, Inc., Chelsea, MI, USA.</p> <p>Sears J and Turchette N (1982). Plasticizers, In: Kirk-Othmer Encyclopedia of Chemical Technology, Eds. Mark H, Othmer D, Overberger C and Seaborg G. Vol. 18, 3rd Edition. John Wiley and Sons, New York, NY, USA.</p>
Test substance	:	diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability	:	<p>(2) valid with restrictions</p> <p>Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database.</p>
Flag	:	Critical study for SIDS endpoint
05.06.2006		(14)
Value	:	156 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Method	:	<p>The calculated value was determined using MPBPWIN version 1.41, a subroutine within the computer program EPI Suite™ version 3.12. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.</p> <p>The Gold and Ogle Method simply uses the formula</p> $T_m = 0.5839T_b$ <p>where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin.</p> <p>The SMILES notation used in the calculation was:</p> <chem>O=C(c1cccc1C(=O)O)O</chem>
Remark	:	EPI Suite™ is used by the US EPA for estimating chemico-physical properties of substances. However, the melting point calculation in EPIWIN

2. Physico-Chemical Data

Id 3648-20-2

Date 07.12.2006

Test substance : provides erroneously high results for phthalate esters.
Reliability : diundecyl phthalate ester (CAS No. 3648-20-2)
05.06.2006 : (3) invalid

(6)

2.2 BOILING POINT

Value : = 501 °C at 1013 hPa
Decomposition : no
Method : other: calculated
Year : 1999
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : Boiling point calculated by MPBPWIN subroutine in EPI Suite™, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
The SMILES notation used in the calculation was:
O=C(c1cccc1C(=O)O)O

Remark : EPI Suite™ is used by the US EPA for estimating chemico-physical properties of substances.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006

(6)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00000000497 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the values for vapor pressure represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate.
Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for diundecyl phthalate ester

2. Physico-Chemical Data

Id 3648-20-2
Date 07.12.2006

was 653.6 cm³ mol⁻¹.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r² = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r² = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r² = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006

(4)

Value : = .00000000163 hPa at 25 °C

Decomposition : no

Method : other (calculated)

Year : 1999

GLP :

Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : Calculated values using MPBPWIN version 1.41, a subroutine of the computer program EPI SuiteTM version 3.12.
Vapor Pressure estimations performed by MPBPWIN are based on the calculation method of Grain, which uses boiling point for the calculation. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985. Neely W and Blau G (1985) have calculated a vapor pressure of 1.22 x 10⁻⁹ mm Hg.

The SMILES notation used in the calculation was:

O=C(c1cccc1C(=O)O)O

Remark : EPI SuiteTM is used by the US EPA for estimating chemico-physical properties of substances.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)

Reliability : (2) valid with restrictions

The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.06.2006

(6)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : = 10.33 at 25 °C

pH value :

Method : other (calculated)

Year :

GLP :

Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Remark : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications,

handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for octanol-water partitioning represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for diundecyl phthalate ester was 653.6 cm³ mol⁻¹.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r² = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r² = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r² = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006

(4)

Partition coefficient : octanol-water
Log pow : = 11.49 at 25 °C
pH value :
Method : other (calculated)
Year : 1999
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : The value was calculated using KOWWIN version 1.67, a subroutine of the computer program EPI Suite™ version 3.12. Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.

The SMILES notation used in the calculation was:

O=C(c1ccccc1C(=O)O)O

Remark : EPI Suite™ is used by the US EPA for estimating chemico-physical properties of substances.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

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(6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

2. Physico-Chemical Data

Id 3648-20-2
Date 07.12.2006

Solubility in : Water
Value : = .00441 other: ug/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Remark : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for water solubility represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume ($\text{cm}^3 \text{mol}^{-1}$). The Le Bas molar volume used for diundecyl phthalate ester was $653.6 \text{ cm}^3 \text{mol}^{-1}$.

$\text{Log CS(WL)} = -0.012V + 5.8$, $n = 35$ (solubility in water)
 $r^2 = 0.98$, $\text{SE} = 0.39$

$\text{Log CS(AL)} = -0.013V - 1.3$, $n = 15$ (solubility in air)
 $r^2 = 0.87$, $\text{SE} = 0.33$

$\text{Log CS(OL)} = -0.016V + 3.4$, $n = 68$ (solubility in octanol)
 $r^2 = 0.19$, $\text{SE} = 0.41$

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
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(4)

Solubility in : Water
Value : = .00016 other: ug/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year : 1999

2. Physico-Chemical Data

Id 3648-20-2
Date 07.12.2006

GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Method : Water solubility calculated by WSKOWWIN, a subroutine of the computer program EPI Suite™ version 3.12. that is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
The SMILES notation used in the calculation was:
O=C(c1cccc1C(=O)OCCCCCCCCCCC)OCCCCCCCCCCC
Remark : EPI Suite™ is used by the US EPA for estimating chemicophysical properties of substances.
Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

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(6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 3648-20-2
Date 07.12.2006

3.1.1 PHOTODEGRADATION

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : 1 based on intensity of sunlight
Conc. of substance : at 25 °C
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000291 cm³/(molecule*sec)
Degradation : = 50 % after 4.4 hour(s)
Deg. product : not measured
Method : other (calculated)
Year : 1999
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : Calculated values using AOPWIN version 1.91, a subroutine of the computer program EPI Suite™ version 3.12.
Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Remark : 50% degradation after 4.4 hrs or 0.37 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI Suite™, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.
EPI Suite™ is used by the US EPA for estimating chemicophysical properties of substances.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006 (6)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : 7.7 year at 25 °C
t1/2 pH9 : at °C
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPI Suite™ version 3.12., that is based on work for EPA by T. Mill et al.

Remark : EPI Suite™ is used by the US EPA for estimating chemicophysical properties of substances.

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)

3. Environmental Fate and Pathways

Id 3648-20-2
Date 07.12.2006

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
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3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1997

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model to represent a diundecyl phthalate ester were:

MW = 474.7
Temperature = 25C
Water Solubility = 0.0000044 mg/L
Vapor Pressure = 4.97E-7 Pa
Pow = 10.3
Melting Point = -9C

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Result : Soil = 97.7%
Air = 0.0%
Water = 0.0%
Sediment = 2.2%
Suspended sed. = 0.1%
Biota = 0.0%

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
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Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III

3. Environmental Fate and Pathways

Id 3648-20-2
Date 07.12.2006

Year :

Remark : Physicochemical input values for the model to represent diundecyl phthalate ester were:
MW = 474.7
Temperature = 25C
Water Solubility = 0.0000044 mg/L
Vapor Pressure = 4.97E-7 Pa
Pow = 10.3
Melting Point = -9C

Emissions rates used in the calculation:

Compartment Rate (kg/hr)

Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment Half-life (hr)

Air	4.0a
Water	240b
Soil	840c
Sediment	840c

a - as calculated using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04 [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from EBSI (1995) and Boethling (2000): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment).

Result : Using the Mackay Level I calculation, the following distribution is predicted for diundecyl phthalate ester:

Compartment	%Distribution
Air	0.4
Water	5.4
Soil	65.3
Sediment	28.9

Test substance : diundecyl phthalate ester (CAS No. 3648-20-2)
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are

05.06.2006

calculated.

(8)

3.4 MODE OF DEGRADATION IN ACTUAL USE**3.5 BIODEGRADATION**

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Contact time : 28 day(s)
Degradation : = 57.4 (±) % after 28 day(s)
Result : inherently biodegradable
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric
Respirometry Test"
Year : 1994
GLP : no
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C11 alkyl esters (CAS No.
3648-20-2)

Result : The biodegradation half-life <4 weeks. By day 28, 57.4% degradation of the test substance was observed. 10% biodegradation was achieved on approximately day 14 and 50% biodegradation on approximately day 24.

By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. Oxygen uptake of the blanks were within guideline limits. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test substance as calculated using results of an elemental analysis of the test substance.

Test Substance:

Day	% Degradation*
12	3, 4, 3
14	13, 15, 16
21	34, 50, 51
28	42, 64, 66 (mean = 57.4)

Positive Reference Substance (Na Benzoate):

Day	% Degradation*
1	32, 36, 34
2	56, 66, 61
5	76, 89, 82

* replicate data

Test condition : Activated sludge and test medium were combined prior to test substance addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test substance was tested in triplicate, controls and blanks were tested in duplicate.

Test substance (1,2-benzenedicarboxylic acid, di-C11 alkyl esters) concentration was approximately 50 mg/L. The positive control (sodium benzoate) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C.

3. Environmental Fate and Pathways

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	All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Test substance	: 1,2-benzenedicarboxylic acid, di-C11 alkyl esters (CAS No. 3648-20-2)
Conclusion	: The test substance is not readily biodegradable.
Reliability	: (1) valid without restriction This summary is rated a "1" and represents a key study because it followed an OECD standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
Flag	: Critical study for SIDS endpoint
05.06.2006	(7)
Type	: aerobic
Inoculum	: activated sludge, domestic, adapted
Concentration	: 20 mg/l related to Test substance related to
Contact time	: 28 day(s)
Degradation	: = 76 (±) % after 28 day(s)
Result	: inherently biodegradable
Deg. product	:
Method	: other: Shake Flask Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill)
Year	:
GLP	: yes
Test substance	: other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Method	: other: Shake Flask Method/Guideline-USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum - Domestic sewage, soil, and mineral medium. Kinetics - Not Reported Degradation Products - Not Reported Analytical Monitoring - Yes
Result	: Primary degradation was expressed as the loss of initial test substance as determined by chemical analysis. Ultimate biodegradation was expressed as percentage CO2 evolved based on total theoretical CO2. >99% primary degradation 76.0% (sd 2.0) ultimate biodegradation
Test condition	: The inoculum was acclimated for 2 weeks prior to test initiation. The test substance was added to flasks that contained medium and inoculum. The flasks were incubated and shaken in the dark for 28 days. Three replicates for CO2 evolution and 4 replicates for primary degradation were evaluated. CO2 produced was captured in barium hydroxide solution. CO2 produced was measured by titration. Primary biodegradation was determined at the beginning, middle and end of the test period by GC-FID (gas chromatographic flame ionization detection) analysis of the entire contents of one replicate. Glucose (positive control) and blank (control) test systems were also evaluated. The test results were corrected for CO2 produced in the blank test systems. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C. Nominal test concentration = 20mg/L for test substance and glucose.
Test substance	: Diundecyl Phthalate Ester (CAS# 3648-20-2) (1,2-benzenedicarboxylic acid, diundecyl ester) Synonym: DUP No information on purity, but DUP was analytically confirmed to be within commercial specifications.
Conclusion	: The data developed in this study, which used an acclimated inoculum, and the remaining biodegradation data summarized by Staples et al. (1997a), which include both acclimated and unacclimated data, clearly show that high molecular weight phthalate esters, including diundecyl phthalate, biodegrade to a great extent.

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Reliability

: (1) valid without restriction

This summary is rated a "1" because it followed a USEPA standard guideline, which describes a procedure specifically designed to evaluate biodegradation under acclimated conditions, and the results were reviewed for reliability and assessed as valid.

07.12.2006

(14) (16)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	: flow through
Species	: Oncorhynchus mykiss (Fish, fresh water)
Exposure period	: 96 hour(s)
Unit	: mg/l
LC50	: > 1.4
Limit test	:
Analytical monitoring	: yes
Method	: other
Year	: 1975
GLP	: yes
Test substance	: other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Method	: Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial concentration.
Result	: 96 hr LC50 >1.4 mg/L Mean measured values were used in the LC50 calculation. Nominal test concentrations: control, 0.12, 0.25, 0.50, 1.0, and 2.0 µl/L. Mean measured test concentrations: <0.0091, 0.11, 0.20, 0.35, 0.88, and 1.4 mg/L. Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period. % Mortality results at 96 hrs per replicate for control and treatment levels: Conc. (mg/L) Rep1/Rep2 Control 0 / 0 0.11 0 / 0 0.20 0 / 0 0.35 0 / 0 0.88 0 / 0 1.4 0 / 0
Test condition	: Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Fish mean length = 39 mm and mean wet weight = 0.6 g. Test temperature = 11 +/-1 Deg C. The pH ranged from 7.1 to 7.5. The mean dissolved oxygen ranged from 9.8 to 10.0 mg/L. Ranges of total hardness and alkalinity as CaCO3 of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.
Test substance	: Fish were obtained from a Maryland supplier. Diundecyl Phthalate Ester (CAS# 3648-20-2) (1,2-benzenedicarboxylic acid, diundecyl ester)

4. Ecotoxicity

Id 3648-20-2
Date 07.12.2006

Conclusion : Synonym: DUP
Purity: 100% active ingredient
: Test substance is non-toxic to fish at or below its water solubility level.
Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
07.12.2006 (5) (15)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : > .02
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: diundecyl phthalate ester (CAS No. 3648-20-2)

Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.
Statistical methods incorporated the following procedures: Moving average angle, Probit, and Binomial Probability.

Result : 48 hr EC50 >0.022 mg/L (based upon time zero analytical samples; no effects at test substance saturation). Value was recalculated as >0.02 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25 µl/L.

Mean measured test concentrations of time 0 and 48 hr values: <0.0087, 0.015, 0.026, 0.048, 0.064, and 0.095 mg/L.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels in the first test:

Conc. (mg/L) Rep1/Rep2/Rep3

Control	0 / 0 / 20
0.015	0 / 0 / 40
0.026	20 / 60 / 80
0.048	80 / 80 / 100
0.064	100 / 100 / 100
0.095	100 / 100 / 100

More than 50% of the organisms were trapped on the surface in the 4 high

treatment solutions. Consequently, the study was repeated as a limit test using a saturated treatment solution.

% Immobility results at 48 hrs per replicate for control and treatment levels in the second limit test:

Conc. (mg/L) Rep1/Rep2/Rep3

Control 0 / 0 / 0

0.02 0 / 0 / 0

Test condition

Data from the second test are used to characterize the acute toxicity of the test substance.

: Test treatments for the initial test were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the first test:

Test temperature = 21.5 +/- 0.5 Deg C. The pH was 8.2 at initiation and 8.3 on day 2. Dissolved oxygen ranged from 7.6 to 7.9 at initiation and was 7.6 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test treatments for the repeat study were prepared by mixing the test substance and 3 L of dilution water (fortified well water) on a magnetic stirrer for 1 hour at a loading of 9.7 mg/L, with a 50% vortex. After mixing the treatment solution was allowed to stand for 1 hour after which 2.5 L of solution was drained from the bottom of the flask into a glass bottle. The solution was allowed to stand for 24 hours after which 2.0 L was drained from the bottom into the test flasks and samples removed for analysis. Three replicates of five organisms were tested. Test vessels were 250 ml beakers with 200 ml of test solution. Control test vessels were prepared under the same conditions but without test substance. Analytical method was Gas Liquid Chromatography (GLC).

Test substance

Water quality parameters for the second test:

Test temperature = 20 Deg C. The pH was 8.2 at initiation and 8.3 on day 2. Dissolved oxygen ranged from 8.8 to 8.9 at initiation and 8.3 to 8.5 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

: Diundecyl Phthalate Ester (CAS# 3648-20-2)
(1,2-benzenedicarboxylic acid, diundecyl ester)
Synonym: DUP

Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

Conclusion

: Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability

: (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag

07.12.2006

: Critical study for SIDS endpoint

(11) (15)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: Selenastrum capricornutum (Algae)
Endpoint	: other: biomass and growth rate
Exposure period	: 8 day(s)
Unit	: mg/l
NOEC	: = 2.1
EC50	: > 2.1
Limit test	:
Analytical monitoring	: yes
Method	: other
Year	: 1978
GLP	: yes
Test substance	: other TS: diundecyl phthalate ester (CAS No. 3648-20-2)
Method	: Method/Guideline - EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978. Statistical methods - Moving average angle, Probit or Bionomial Test type - Static
Result	: 192 hr (8 day) EC50 >3.3 mg/L (based upon time zero analytical samples). Value was recalculated as >2.10 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997). Mean measured values were used in the final EC50 calculation. Nominal test concentration as a percent of a saturated solution: 0 (control) and 100.0%. Mean measured test concentrations of time 0 and 144 hr values: <0.05 and 2.10 mg/L (detection limit was 0.05 mg/L). Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect of 10 and 22% as compared with the control for chlorophyll a was measured on days 6 and 8, respectively. Analytical samples were taken at time zero and on a composite of replicates at termination. Chlorophyll a percent change relative to control on sampling days and cell number on day 8 results: Conc. Chlorophyll a percent change from control (mg/L) Day 1 Day 2 Day 4 Day 6 Day 8 Cell # Day 8 2.10 -3 -4 -3 +10 +22 +12
Test condition	: Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100% WSF) because earlier phthalate testing suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility. Lighting = 4,700 lux, Test temperature = 22+/-2 Deg C. The pH was 7.5 at initiation and 8.3 on day 8. Algal culture stock was obtained from University of Texas at Austin, TX.
Test substance	: Diundecyl Phthalate Ester (CAS# 3648-20-2) (1,2-benzenedicarboxylic acid, diundecyl ester) Synonym: DUP Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.

Conclusion	: Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al (1997).
Reliability	: (1) valid without restriction The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances. Control chlorophyll or cell counts not reported.
Flag 07.12.2006	: Critical study for SIDS endpoint (12) (15)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)																									
Endpoint	:	reproduction rate																									
Exposure period	:	21 day(s)																									
Unit	:	mg/l																									
NOEC	:	= .9																									
EC50	:	> .9																									
Analytical monitoring	:	yes																									
Method	:	OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"																									
Year	:	1984																									
GLP	:	yes																									
Test substance	:	other TS: Diundecyl Phthalate Ester (CAS No. 3648-20-2)																									
Method	:	The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.																									
Result	:	Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Diisoundecyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.																									
		<table><tr><td></td><td>Control</td><td>Dispersant</td><td>Control</td><td>Test Substance</td></tr><tr><td>Po % Mortality</td><td>0</td><td>20</td><td></td><td>0</td></tr><tr><td>Mean F1/</td><td></td><td></td><td></td><td></td></tr><tr><td>Surviving Po</td><td>120 (sd=13.3)</td><td>131 (sd=23.5)</td><td>134 (sd=20.9)</td><td></td></tr><tr><td>Po Mean Length</td><td>4.2 (sd=0.14)</td><td>4.3 (sd=0.16)</td><td>4.3 (sd=0.17)</td><td></td></tr></table>		Control	Dispersant	Control	Test Substance	Po % Mortality	0	20		0	Mean F1/					Surviving Po	120 (sd=13.3)	131 (sd=23.5)	134 (sd=20.9)		Po Mean Length	4.2 (sd=0.14)	4.3 (sd=0.16)	4.3 (sd=0.17)	
	Control	Dispersant	Control	Test Substance																							
Po % Mortality	0	20		0																							
Mean F1/																											
Surviving Po	120 (sd=13.3)	131 (sd=23.5)	134 (sd=20.9)																								
Po Mean Length	4.2 (sd=0.14)	4.3 (sd=0.16)	4.3 (sd=0.17)																								
Test condition	:	Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.																									
		Ten replicate test systems with 1 daphnid each (< 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.																									

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The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:

Temperature = 20 +/- 1.0 degree C
Water hardness = >140 mg/L (as CaCO₃)
Alkalinity = >100 mg/L (as CaCO₃)
pH = approximately 8
Dissolved oxygen = 8-9 mg/L

Standard daily feeding rates with the cultured alga, *Chlorella vulgaris*, was supplemented with microencapsulated food, "Frippak Booster". This rate was increased by 10% from day 5 of the test as data from earlier studies indicated that additional feed was appropriate to prevent stress due to food deficiency.

Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations were 0.91 mg/L in new exposure solutions and 0.90 mg/L in old exposure solutions, which represents 91 and 90%, respectively, of the nominally added test substance.

Test substance Conclusion

: Diundecyl Phthalate Ester (CAS No. 3648-20-2); purity >99.5%
: Chronic invertebrate (*Daphnia magna*) toxicity data reported for diisoundecyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisoundecyl phthalate ester, do not produce chronic toxicity to *Daphnia magna*. Testing was conducted at a loading that exceeds the water solubility of diisoundecyl phthalate ester (expected to be less than 0.17 ug/L, which was determined for a diisodecyl phthalate ester; Letinski et al., 2002) after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.

Reliability

: (1) valid without restriction
The study procedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag
07.12.2006

: Critical study for SIDS endpoint

(3)

Species
Endpoint
Exposure period
Unit
NOEC
EC50
Analytical monitoring
Method
Year
GLP
Test substance

: *Daphnia magna* (Crustacea)
: reproduction rate
: 21 day(s)
: mg/l
: = .059
: > .059
: yes
: other
: 1982
: yes
: other TS: Diundecyl Phthalate Ester (CAS No. 3648-20-2)

Method

: The test method is in general agreement with US EPA Environmental Effects Test Guidelines, ES-1, EPA 560/6-82-002.

Result

: *Daphnia* adult survival and reproduction (cumulative number of offspring per live adult) were evaluated as the biological endpoints. Diundecyl phthalate showed no effect on survival or reproduction at its highest

Test condition	<p>achievable water solubility (0.059 mg/L) under the conditions of this test.</p> <p>: The study used a flow-through test system. The test systems used modified proportional diluters with a 0.5 dilution factor to deliver exposure solutions. Test substance exposure solutions were prepared using a gas-tight syringe with a mechanical injector that introduced the appropriate volume of test substance into a mixing chamber during each exposure level diluter cycle. Control systems received no test substance. From the mixing chamber, exposure solutions then flowed to the test systems.</p> <p>Four replicate test systems with 20 daphnids each (\leq 24 hours old) were used for each test substance concentration. Test systems were 1.75 L glass battery jars. Test and control solutions drained from the test systems through a 3.5x8.0 cm notch that was located at the upper edge of the test system. The notch in each test system was covered with 40-mesh Nitex screen to prevent the loss of daphnids. The diluters delivered 50 ml of test solution to each test system at a rate equivalent to 4.4 to 5.0 volume replacements daily. Illumination, 2 to 4 hectolux (2.94 to 5.88 Wm⁻²) at the solution surface, of the test systems was provided by Durotest (Optima) fluorescent lights, which were located above the test systems.</p> <p>The dilution water used for the tests and the culture was well water to which selected salts were added to achieve specific water quality ranges. Water quality measurements including dissolved oxygen concentration and temperature were determined every weekday within one replicate test chamber of each treatment level and control. Total hardness, alkalinity, specific conductance, and pH were monitored weekly in one test vessel from each treatment and control. Test conditions were:</p> <p style="padding-left: 40px;">Temperature = 21 \pm 2.0 degree C Water hardness = 150 to 180 mg/L (as CaCO₃) Alkalinity = 100 to 130 mg/L (as CaCO₃) pH = 7.9 to 8.3 Dissolved oxygen > 60% saturation Specific conductance = 400 to 600 μmho/cm</p> <p>Adult survival and offspring production by daphnids were assessed every weekday from day 7 through day 21. The offspring were removed, counted, and discarded, and the adults were returned to their respective test systems after each system had been brushed to remove algal growth. Food was placed in the test systems three times a day during weekdays and twice daily on weekends. A feeding consisted of a 2.0 ml of a salmon starter solution prepared at 5.0 mg/ml, followed with 2.0 ml of an alga suspension containing <i>Selenastrum</i> sp., <i>Ankistrodesmus</i> sp., and <i>Chlamydomonas</i> sp. at concentrations of 1×10^7 to 5.0×10^7 each.</p>
Test substance Conclusion	<p>Test substance analyses of exposure solutions were performed using gas chromatography. The mean measured water exposure concentrations were: control (below minimum detectable level), 0.004 (SD 0.001), 0.008 (SD 0.001), 0.014 (SD 0.003), 0.028 (SD 0.005), 0.059 (SD 0.011).</p> <p>: Diundecyl Phthalate Ester (CAS No. 3648-20-2)</p> <p>: The chronic invertebrate (<i>Daphnia magna</i>) toxicity data reported for diundecyl phthalate are consistent with the data for several high molecular weight phthalate esters as summarized by Rhodes et al. (1995). These data clearly showed that high molecular weight phthalate esters, including diundecyl phthalate, did not produce chronic toxicity to an invertebrate at or below their maximum attainable water solubility.</p>
Reliability	<p>: (1) valid without restriction</p> <p>The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.</p>

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(10) (13)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY****5.1.2 ACUTE INHALATION TOXICITY****5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES****5.2.1 SKIN IRRITATION****5.2.2 EYE IRRITATION****5.3 SENSITIZATION****5.4 REPEATED DOSE TOXICITY**

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	oral feed
Exposure period	:	21 days
Frequency of treatm.	:	Continuous
Post exposure period	:	None
Doses	:	0, 0.3, 1.2, 2.5% (~0, 282, 1145, and 2305 mg/kg/day)
Control group	:	yes, concurrent no treatment
NOAEL	:	= 282 - mg/kg bw
Method	:	other
Year	:	1985
GLP	:	no data
Test substance	:	other TS: Diundecyl Phthalate Ester (CAS No. 3648-20-2)
Method	:	Statistical methods: not available
Result	:	NOAEL = 0.3% (approximately 282 mg/kg/day), based on decreased body weight gains and increased liver weights. Statistically significant decreases in body weight gain were observed at the mid and high dose for males and females. Slight changes in food consumption for both sexes were also observed; however, these changes were not statistically significant. At the mid and high dose, liver, and kidney weights were increased. In addition, increases were seen in liver enzymes and palmitoyl-CoA oxidation (an indicator of peroxisome proliferation. Mid- and high-dose males also had increased relative testes weight, but no lesions were observed histopathologically.
Test condition	:	Rats (n=5/sex/dose) were randomly assigned to the treatment groups. Following the acclimation period, the test or control diets were given to the

5. Toxicity

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rats for 21 days. The females received the test diets one day later than the males to allow the male and female necropsies to be conducted on consecutive days.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate)
CAS # 3648-20-2

Conclusion : The test substance was "mildly hepatotoxic" at levels of 1.2% and 2.5% in the diet of male rats.

Reliability : (2) valid with restrictions
Limited hematological and serum chemistry endpoints evaluated.

Flag : Critical study for SIDS endpoint
07.12.2006 (2)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : Salmonella typhimurium /TA98; TA100; TA1535; TA1537

Test concentration : 5 dose levels up to 10 mg/plate

Cycotoxic concentr. :

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471

Year : 1985

GLP : no data

Test substance : other TS: Diundecyl Phthalate Ester (CAS No. 3648-20-2)

Method : A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.

Test condition : Approximately 108 bacteria were mixed with 0.5 ml of either 0.1M sodium phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest was conducted to determine the high dose level. This study was conducted with TA100 in the presence and absence of S-9.

Test substance : 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate)
CAS # 3648-20-2

Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA98, TA100, TA1535 and TA1537 with or without metabolic activation.

Reliability : (1) valid without restriction
NTP-sponsored study.

Flag : Critical study for SIDS endpoint
07.12.2006 (17)

Type : Mouse lymphoma assay

System of testing : Mouse lymphoma cells/L5178Y.

Test concentration : 1 to 10 µl/ml

Cycotoxic concentr. : 10 µl/ml

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 476

Year : 2000

GLP : yes

Test substance : other TS: 711P

Method	: Metabolic Activation: With and without Arochlor-induced rat liver S9 mixture.
	Control Groups: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9.
	Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10×10^{-6} . The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	: Cytotoxicity ranged from 3.5 - 21% at the high dose levels. In the absence of activation, 2 to 10 ul/ml induced moderate to high toxicity (percent relative growths: 18.8% to 70.7%), but no increase in mutation frequency. In the presence of a metabolic fraction, 1 to 8 ul/ml was toxic (percent relative growths: 3.5% to 62.7%), without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic with activation in this assay.
Test condition	: Mouse lymphoma cells were seeded into a series of tubes at 6×10^6 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3×10^6 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony counts at each dose level were determined by triplicate plates.
Test substance	: Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11).
	Data used as read-across to 3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (diundecyl phthalate)
Conclusion	: Under conditions of this study diundecyl phthalate was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
06.07.2006	(1)

5.6 GENETIC TOXICITY 'IN VIVO'**5.7 CARCINOGENICITY****5.8.1 TOXICITY TO FERTILITY****5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY****5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES**

5. Toxicity

Id 3648-20-2
Date 07.12.2006

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 3648-20-2
Date 07.12.2006

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY**10.2 HAZARD SUMMARY**

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physicochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

06.07.2006

10.3 RISK ASSESSMENT